Energy Frontier Research Centers

Tackling Our Energy Challenges in a New Era of Science

The Department of Energy's Office of Science, Office of Basic Energy Sciences announces the initiation of Energy Frontier Research Centers (EFRCs) to accelerate the rate of scientific breakthroughs needed to create advanced energy technologies for the 21st century. The EFRCs will pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical energy.

Background Information

Context. Imagine a virtually unlimited supply of electrical power from solar-energy systems, modeled on the photosynthetic processes utilized by green plants, and power lines that could transmit this electricity from the deserts of the southwest to the Eastern Seaboard at nearly 100 percent efficiency. If the technological advances in information of the 20th century serve as a guide, disruptive advances borne out of pushing the science frontiers will be a key to addressing 21st century energy challenges.

Establishing the Energy Research Directions. In 2001, the Basic Energy Sciences Advisory Committee (BESAC) conducted a far reaching study to assess the scope of fundamental scientific research that must be considered to address the DOE missions in energy efficiency, renewable energy resources, improved use of fossil fuels, safe and publicly acceptable nuclear energy, future energy sources, and reduced environmental impacts of energy production and use.

The scientific community responded to this BESAC study with enthusiasm through participation in a week-long workshop, whose results were published in early 2003 in the report, *Basic Research Needs to Assure a Secure Energy Future*. That report inspired a series of ten follow-on "*Basic Research Needs*" workshops over the next five years, which together attracted more than 1,500 participants from universities, industry, and DOE laboratories. Topics included the hydrogen economy; solar energy utilization; superconductivity; solid-state lighting; advanced nuclear energy systems; combustion of 21st century transportation fuels; electrical-energy storage; geosciences as it relates to the storage of energy wastes (the long-term storage of both nuclear waste and CO_2); materials under extreme environments; and catalysis for energy-related processes. Amongst these reports, research needs in theory, modeling, and simulation have been a central theme, in which the BESAC report, *Opportunities for Discovery: Theory and Computation in Basic Energy Sciences*, captures major highlights.

The New Era of Science. Together, these workshop reports highlighted the remarkable scientific journey that has taken place during the past few decades. The resulting scientific challenges, which no longer were discussed in terms of traditional scientific disciplines, described a new era of science – an era in which materials functionalities are designed to specifications and chemical transformations are manipulated at will. Over and over, the recommendations from the workshops described similar themes – that in this new era of science, we would design, discover, and synthesize new materials and molecular assemblies through atomic scale control; probe and control photon, phonon, electron, and ion interactions with matter; perform multi-scale modeling that bridges the multiple length and time scales; and use the collective efforts of condensed matter and materials physicists, chemists, biologists, molecular engineers, and those skilled in applied mathematics and computer science.

The Grand Science Challenges. To accomplish this—to direct and control matter at the quantum, atomic, and molecular levels—requires a change in our fundamental understanding of how nature works. A BESAC Grand Challenges subcommittee was convened, which examined the roadblocks to progress, and the opportunities for truly transformational new understanding. The results of that examination were presented in the report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*. This new era of energy science poses five challenges:

- How do we control materials processes at the level of electrons?
- How do we design and perfect atom- and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
- How do we characterize and control matter away—especially very far away—from equilibrium?

Addressing these grand challenges is key to making the transition from observation to control of matter.

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To implement the collective recommendations of these twelve workshops, the Office of Basic Energy Sciences announces a new initiative: the Energy Frontier Research Centers (EFRCs). The EFRC awards are expected to be in the $2–5 million range annually for an initial 5-year period. A Funding Opportunity Announcement (FOA) will be issued in FY 2008 to request applications from the scientific community for the establishment of the initial suite of EFRCs. It is anticipated that approximately $100 million will be available for multiple EFRC awards starting in FY 2009.

Distinguishing Attributes. Energy Frontier Research Centers will bring together the skills and talents of multiple investigators to enable research of a scope and complexity that would not be possible with the standard individual investigator or small group award. An EFRC will have the following characteristics:

- The research program is at the forefront of one or more of the challenges described in the BESAC report *Directing Matter and Energy: Five Challenges for Science and the Imagination* (http://www.sc.doe.gov/bes/reports/files/GC_rpt.pdf).
- The research program addresses one or more of the energy challenges described in the ten BES workshop reports in the *Basic Research Needs* series (http://www.sc.doe.gov/bes/reports/list.html).
- The program is balanced and comprehensive, and, as needed, supports experimental, theoretical, and computational efforts and develops new approaches in these areas.
- The program provides opportunities to inspire, train, and support leading scientists of the future who have an appreciation for the global energy challenges of the 21st century.

- The center leadership communicates effectively with scientists of all disciplines and promotes awareness of the importance of energy science and technology.
- There is a comprehensive management plan for a world-leading program that encourages high-risk, high-reward research. The Center's management plan demonstrates that the whole is substantially greater than the sum of the individual parts.

Research Focus Areas. EFRC proposals must address all of the attributes listed above. A few examples of science areas that would respond to the solicitation are given below. These are intended to be examples only. The intent of the program is to allow for maximum flexibility within the broad guidelines given above. We are particularly interested in tapping the imagination and creativity of the scientific community to address the fundamental questions of how nature works and to harness this new knowledge for some of our most critical real-world challenges.

- ***Direct conversion of solar energy to electricity and chemical fuels.*** Learning to direct and control materials and chemical processes at the level of electrons, where the laws of quantum mechanics rule, would pave the way for essentially new quantum control impacting catalysis, photochemistry, molecular biology, and device physics that are the foundational pieces in solar energy conversion. Powerful new methods of nanoscale fabrication, characterization, and simulation—using physical, chemical and biological tools that were not available as few as five years ago—create new opportunities for understanding and manipulating the molecular and electronic pathways of solar energy conversion. Specific areas include coaxing cheap materials for superior performance; new paradigms for solar cell design; photo-catalytic processes for inexpensive, efficient conversion; and bio-inspired methods for self-assembly of molecular components into functional self-regulating, and self-repairing systems for solar fuel production.

- ***Understanding of how biological feedstocks are converted into portable fuels***[1] Biological systems are the proof-of-concept for what can physically be achieved by nanotechnology. Consider the ease with which biological systems transform and store energy or their ability to self-repair and to adapt to changing external conditions. The way in which energy, entropy, and information are manipulated within the nanosytems of life provides us with lessons on what we must learn in order to develop similarly sophisticated energy technologies. This entails research in light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide as well as carbon fixation and storage. Specific areas might include molecular-scale characterization of the physical structure and chemical properties of plant cell wall materials with the aim of circumventing the need for extensive pre-treatment and biological hydrolysis to sugars (saccharification), which are current bottlenecks in cellulosic biofuel production. Other areas include development of new and improved catalytic conversion processes that are far more robust than enzymatic systems for the conversion of plant polymers to fuels.

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[1] Within the Office of Science, both the BES and the Biological and Environmental Research (BER) programs' biofuels research involve the direct biological conversion of solar energy into chemically stored fuels. However, there are distinct differences. BES focuses on the conversion mechanisms, emphasizing the associated physical, chemical processes, and their coupling with bio- and biomimetic approaches. In contrast, BER focuses on the biological processes, with an emphasis on genomics, metabolic engineering, systems biology, and biotechnological tools for scalable biofuels production. BES biofuels research also emphasizes utilization of physical sciences-based theoretical and experimental tools and combines them with existing biochemical and molecular biological tools to probe energy transduction and chemical energy deposition processes.

- ***A new generation of radiation-tolerant materials and chemical separation processes for fission applications.*** By designing and perfecting atom- and energy-efficient synthesis, one can create a paradigm shift in the discovery and design of new chemical assemblies and materials that are mechanical strong; light weight; and resistant to corrosion, decay, or failure in extreme conditions of temperature, pressure, radiation, or chemical exposures encountered in fission applications. Key research includes: foundational research in chemistry and physics of actinides and their fission products; new generation of actinide separations processes with improved efficiency, selectivity, cost-effectiveness, and waste minimization; first-principles design and understanding of materials with improved radiation and corrosion resistance at elevated temperatures; microstructural design and predictive models for mitigating long-time degradation behavior; characterization, theory, and computer models for decades-to-centuries performance; and solution and interfacial behavior under extreme radiation flux and elevated temperatures.

- ***Addressing fundamental knowledge gaps in energy storage.*** Without effective electrical energy storage, renewable—yet intermittent—sources of energy such as wind and solar will not be able to significantly displace fossil, nuclear, and other conventional energy sources used for generating electricity for the power grid. Similarly, current battery technologies are limited, making plug-in hybrid or all-electric cars prohibitively costly and insufficient to meet consumer demands. Long-term, fundamental research in electrical energy storage will be needed to accelerate the pace of scientific discoveries and to see transformational advances that bridge the gaps in cost and performance, separating the current technologies and those required for future utility and transportation needs. For example, by mastering energy balance on the nanoscale through harvesting the large number of forces that are often operating simultaneously, such as electrostatic attraction and repulsion, chemical bonding, surface tension, and random forces from environmental fluctuations, a wide variety of structures can be assembled for 3-D architectures with multi-functionalities in energy storage unsurpassed by any given existing technologies. Other research areas include new capabilities to "observe" the dynamic composition and structure of the constituents in the electrochemical storage systems; novel electrolytes with high conductivity over a broad temperature range and long-term stability; and theory, modeling, and simulation that integrate methods at different time and length scales.

- ***Transforming energy utilization and transmission.*** At the heart of the nanoscale behavior, one often finds emergent phenomena, in which a complex outcome emerges from the correlated interactions of many simple constituents. By understanding the fundamental rules of correlations and emergence and then by learning how to control them, we could produce, for example, an entirely new generation of energy utilization and transmission processes, such as in phase change materials for thermal energy conversion, strong light-matter interaction and collective charge behavior for light emission nearing theoretical efficiency, and radically different combustion chemistry of alternative fuels. Understanding the emergent behavior of materials and chemical reactivity at the nanoscale offers remarkable opportunities in broad arena of applications including solid-state lighting, electrical generators, clean and efficient combustion of 21st century transportation fuels, catalytic processes for efficient production and utilization of chemical fuels, and superconductivity for resistance-less electricity transmission.

- ***Science-based geological carbon sequestration.*** All natural and most human-induced phenomena occur in systems that are away from the equilibrium in which the system would not change with time. If we can understand system effects that take place away—especially very far away—from equilibrium and learn to control them, it could yield dramatic new carbon capture technologies and enable new strategies for sequestering carbon to mitigate environmental damage. Key research areas involve new membranes and separations of carbon dioxide from process streams at high temperature and pressure; understanding geochemical processes relevant to the dimensions of subsurface sequestration sites with realistic geological formations chemistry; developing critical geophysical measurement techniques for remote probing and tracking; developing fluid-flow measurement approaches and simulation tools that can link chemical and physical processes at multiple scales; and advanced measurement and modeling verification at field sites.

EFRC Awards Process. A number of EFRC awards will be initiated in FY 2009 based on an open competition among academic institutions, DOE laboratories, and other institutions. Research activities may be sited at universities, at DOE laboratories, or in joint university-laboratory collaborations. The EFRC awards are expected to be in the $2–5 million range annually for an initial 5-year period. A Funding Opportunity Announcement (FOA) will be issued in FY 2008 to request applications from the scientific community for the establishment of the initial suite of EFRCs. It is anticipated that approximately $100 million will be available for multiple EFRC awards. As the EFRC program matures, it is anticipated that EFRC competitions will be held every 2 or 3 years and that renewal submissions will be openly competed with new submissions. Out-year funding is subject to satisfactory progress in the research and the availability of funding appropriations. While capital investment in instrumentation and infrastructure are expected as part of the EFRC awards, usage and leverage of existing facilities, including the BES user facilities, is encouraged. This announcement, updates, and further information on the FOA will be available through a link on the BES home page (http://www.sc.doe.gov/bes/).